Soft Confinement of Self-Propelled Rods: Simulation and Theory

Supplementary Material

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1 Potential Energy of a Discrete Rod in an External Field

In this section, we derive the effective potential energy a rod center of mass experiences at a given position and orientation. This derivation applies to rods made of a discrete number of point masses separated by distance σ. In the thin rod limit, we show that the energy for a discrete rod matches the continuous solution described in the main text.

For a rod made of N_s monomers spaced at distance σ, the potential acting on each **monomer** can be described by a Fourier series.

$$\phi(\mathbf{r}_i) = \frac{1}{N_s} \sum_{n,m} \hat{\phi}_{nm} e^{i2\pi \mathbf{k}_{nm} \cdot \mathbf{r}_i} \tag{1}$$

The position of each monomer on the rod can be described by:

$$\mathbf{r}_i = \mathbf{r} + s_i \sigma \mathbf{u} \tag{2}$$

where $\mathbf{u} = \{\cos(\theta), \sin(\theta)\}^T$ is the orientation vector describing the direction to step away from the rod center of mass $\mathbf{r}$. s_i is an integer counting the number of monomer units away from the center of mass. For example, provided there are an odd number of monomers:

$$s = -\frac{N_s - 1}{2}, ..., \text{-}3, \text{-}2, \text{-}1,\ 0\ ,\ 1,\ 2,\ 3, ...,\ \frac{N_s - 1}{2}$$

The potential energy of the entire rod is then:

$$V_{Rod}(\mathbf{r}, \theta) = \sum_{i}^{N_s} \frac{1}{N_s} \sum_{n,m} \hat{\phi}_{nm} e^{i2\pi \mathbf{k}_{nm} \cdot (\mathbf{r} + s_i \sigma \mathbf{u})} \tag{3}$$

Except for $s_i = 0$ there are $(N_s - 1)/2$ pairs of beads on opposite sides of the center of mass: $s_i = \pm 1, \pm 2, ..., \pm (N_s - 1)/2$. Using the angle sum/difference formula we can describe the pairs as

$$e^{i2\pi \mathbf{k}_{nm} \cdot (\mathbf{r} + s_i \sigma \mathbf{u})} + e^{i2\pi \mathbf{k}_{nm} \cdot (\mathbf{r} - s_i \sigma \mathbf{u})} = 2 e^{i2\pi \mathbf{k}_{nm} \cdot \mathbf{r}} \cos(2\pi \mathbf{k}_{nm} \cdot s_i \sigma \mathbf{u}). \tag{4}$$

Simplifying the sum provides the following expression:

$$V_{Rod}(\mathbf{r}, \theta) = \frac{1}{N_s} \sum_{n,m} \hat{\phi}_{nm} e^{i2\pi \mathbf{k}_{nm} \cdot \mathbf{r}} \left[1 + 2 \sum_{s_i=1}^{s_i=(N_s-1)/2} \cos(2\pi \mathbf{k}_{nm} \cdot s_i \sigma \mathbf{u}) \right] \tag{5}$$

The inner series can be solved exactly via telescopic sums:

$$S_M = 2 \sum_{s_i=1}^{s_i=(N_s-1)/2} \cos(2\pi \mathbf{k}_{nm} \cdot s_i \sigma \mathbf{u}) \tag{6a}$$

$$S_M = \csc(\pi \mathbf{k}_{nm} \cdot \sigma \mathbf{u}) \sin(N_s \pi \mathbf{k}_{nm} \cdot \sigma \mathbf{u}) - 1 \tag{6b}$$

Plugging this into the Eq. 5 gives the potential energy of a rod made of N_s monomers separated by distance σ in an external field.

$$V_{Rod}(\mathbf{r}, \theta) = \frac{1}{N_s} \sum_{n,m} \hat{\phi}_{nm} e^{i2\pi \mathbf{k}_{nm} \cdot \mathbf{r}} \csc\left(\pi \sigma \mathbf{k}_{nm} \cdot \mathbf{u}\right) \sin\left(\pi N_s \sigma \mathbf{k}_{nm} \cdot \mathbf{u}\right) \tag{7}$$

The discrete solution matches the continuous solution when $N_s = \sigma^{-1} L_{Rod}$, and $\sigma \to 0^+$

$$\lim_{\sigma \to 0^+} \frac{\sigma}{L_{Rod}} \csc\left(\pi \sigma \mathbf{k}_{nm} \cdot \mathbf{u}\right) \sin\left(\pi L_{Rod} \mathbf{k}_{nm} \cdot \mathbf{u}\right) = \operatorname{sinc}\left(\pi L_{Rod} \mathbf{k}_{nm} \cdot \mathbf{u}\right). \tag{8}$$

The convergence of the limit can be found by the Taylor series expansion around $\sigma \to 0^+$

$$\lim_{\sigma \to 0^+} \frac{\sigma}{L_{Rod}} \csc\left(\pi \sigma \mathbf{k}_{nm} \cdot \mathbf{u}\right) \sin\left(\pi L_{Rod} \mathbf{k}_{nm} \cdot \mathbf{u}\right) = \operatorname{sinc}\left(\pi L_{Rod} \mathbf{k}_{nm} \cdot \mathbf{u}\right) * \left(1 + \frac{\left(\sigma \pi \mathbf{k}_{nm} \cdot \mathbf{u}\right)^2}{6} + + \frac{7\left(\sigma \pi \mathbf{k}_{nm} \cdot \mathbf{u}\right)^4}{360} + \mathscr{O}(\sigma^6)\right) \tag{9}$$

2 Taylor Dispersion Theory for Active Rods

The general Smoluchowski equation for a thin active rod moving at a constant swim velocity U_0 under an external potential field $V(\mathbf{x}, \mathbf{r}, \theta, t)$ is given as:

$$\frac{\partial P(\mathbf{x}, \mathbf{r}, \theta, t)}{\partial t} + (\nabla_x + \nabla_r) \cdot \mathbf{J_T} + + \frac{\partial}{\partial \theta} J_\theta = 0 \tag{10a}$$

$$\mathbf{J_T} = \left[U_0 \mathbf{u} P - \mathbf{D}(\mathbf{u}) \cdot \left((\nabla_x + \nabla_r) P + P(\nabla_x + \nabla_r) \left[\frac{V}{k_\mathrm{B} T}\right]\right)\right] \tag{10b}$$

$$J_\theta = -D_\theta \left(\frac{\partial}{\partial \theta} P + P \frac{\partial}{\partial \theta} \left[\frac{V}{k_\mathrm{B} T}\right]\right) \tag{10c}$$

Where $\mathbf{x}$ is the lattice vector denoting global position, $\mathbf{r}$ is the local vector denoting position inside a periodic cell, θ is the rod orientation angle, $\mathbf{u} = [\cos(\theta), \sin(\theta)]^T$ is the orientation unit vector, and t is time. $k_\mathrm{B} T$ is the thermal energy and $\mathbf{D}(\mathbf{u})$ is the orientationally dependent diffusivity tensor. Assuming the potential is constant between lattices. $\nabla_x \left[\frac{V}{k_\mathrm{B} T}\right] = \mathbf{0}$. We simplify the equation and then take the Fourier transform over the lattice vector $\mathbf{x} \to \mathbf{k}$.

$$\frac{\partial \hat{P}(\mathbf{k}, \mathbf{r}, \theta, t)}{\partial t} + (i\mathbf{k} + \nabla_r) \cdot \hat{\mathbf{J}}_T + \frac{\partial}{\partial \theta} \hat{J}_\theta = 0 \tag{11a}$$

$$\hat{\mathbf{J}}_T(\mathbf{k}, \mathbf{r}, \theta, t) = \left[U_0 \mathbf{u} \hat{P} - \mathbf{D}(\mathbf{u}) \cdot \left((i\mathbf{k} + \nabla_r) \hat{P} + \hat{P} \nabla_r \left[\frac{V}{k_\mathrm{B} T}\right]\right)\right] \tag{11b}$$

$$\hat{J}_\theta(\mathbf{k}, \mathbf{r}, \theta, t) = -D_\theta \left(\frac{\partial}{\partial \theta} \hat{P} + \hat{P} \frac{\partial}{\partial \theta} \left[\frac{V}{k_\mathrm{B} T}\right]\right) \tag{11c}$$

Define the macroscopic number density $\hat{n}(\mathbf{k}, t) = \langle \hat{P} \rangle_{\theta, r}$, and then take the orientational and local position average of Eq. 11. $\langle f \rangle_q$ is the integral of f over coordinate q.

$$\frac{\partial \hat{n}}{\partial t} + i\mathbf{k} \cdot \left\langle \hat{\mathbf{J}}_T \right\rangle_{\theta, r} + \left\langle \nabla_r \cdot \hat{\mathbf{J}}_T \right\rangle_{\theta, r} + \left\langle \frac{\partial}{\partial \theta} \hat{J}_\theta \right\rangle_{\theta, r} = 0 \tag{12}$$

From the divergence theorem, we know that $\left\langle \nabla_r \cdot \hat{\mathbf{J}}_T \right\rangle_{\theta, r} = 0$ and $\left\langle \frac{\partial}{\partial \theta} \hat{J}_\theta \right\rangle_{\theta, r} = 0$.

2.0.1 General Fourier Transformed Macroscopic Number Density Equation

$$\frac{\partial \hat{n}(\mathbf{k}, t)}{\partial t} + i\mathbf{k} \cdot \left\langle \hat{\mathbf{J}}_T \right\rangle_{\theta, r} = 0 \tag{13a}$$

$$\left\langle \hat{\mathbf{J}}_T \right\rangle_{\theta, r} = \left[U_0 \left\langle \mathbf{u} \hat{P} \right\rangle_{\theta, r} - \left\langle \mathbf{D}(\mathbf{u}) \cdot \left((i\mathbf{k} + \nabla_r) \hat{P} + \hat{P} \nabla_r \left[\frac{V}{k_\mathrm{B} T}\right]\right)\right\rangle_{\theta, r}\right] \tag{13b}$$

2.1 Assuming isotropic diffusivity

Assuming $\mathbf{D}(\mathbf{u}) = D_T\mathbf{I}$ The Fourier Transformed Smoluchowski equation is:

$$\frac{\partial \hat{P}(\mathbf{k},\mathbf{r},\theta,t)}{\partial t} + (i\mathbf{k}+\nabla_r)\cdot\hat{\mathbf{J}}_T + \frac{\partial}{\partial\theta}\hat{J}_\theta = 0 \tag{14a}$$

$$\hat{\mathbf{J}}_T(\mathbf{k},\mathbf{r},\theta,t) = \left[U_0\mathbf{u}\hat{P} - D_T\left((i\mathbf{k}+\nabla_r)\hat{P} + \hat{P}\nabla_r\left[\frac{V}{k_{\mathrm{B}}T}\right]\right)\right] \tag{14b}$$

$$\hat{J}_\theta(\mathbf{k},\mathbf{r},\theta,t) = -D_\theta\left(\frac{\partial}{\partial\theta}\hat{P} + \hat{P}\frac{\partial}{\partial\theta}\left[\frac{V}{k_{\mathrm{B}}T}\right]\right) \tag{14c}$$

And the macroscopic density is:

$$\frac{\partial \hat{n}(\mathbf{k},t)}{\partial t} + i\mathbf{k}\cdot\left\langle\hat{\mathbf{J}}_T\right\rangle_{\theta,r} = 0 \tag{15a}$$

$$\left\langle\hat{\mathbf{J}}_T\right\rangle_{\theta,r} = \left[U_0\left\langle\mathbf{u}\hat{P}\right\rangle_{\theta,r} - D_T\left(i\mathbf{k}\left\langle\hat{P}\right\rangle_{\theta,r} + \left\langle\nabla_r\hat{P}\right\rangle_{\theta,r} + \left\langle\hat{P}\nabla_r\left[\frac{V}{k_{\mathrm{B}}T}\right]\right\rangle_{\theta,r}\right)\right] \tag{15b}$$

We define the Fourier transformed structure function in terms of the Fourier transformed probability and macroscopic density $\hat{G}(\mathbf{k},\mathbf{r},\theta,t) = \hat{P}/\hat{n}$. We multiply Eq. 15 by $\hat{G}$ and subtract from Eq. 11

$$\frac{\partial\hat{P}}{\partial t} - \hat{G}\frac{\partial\hat{n}}{\partial t} + i\mathbf{k}\cdot\left(\hat{\mathbf{J}}_T - \hat{G}\left\langle\hat{\mathbf{J}}_T\right\rangle_{\theta,r}\right) + \nabla_r\cdot\hat{\mathbf{J}}_T + \frac{\partial}{\partial\theta}\hat{J}_\theta = 0 \tag{16}$$

Now divide the equation by $\hat{n}$, recognizing that from the chain rule acting on $\hat{P} = \hat{G}\hat{n}$ gives $\frac{\partial\hat{P}}{\partial t} - \hat{G}\frac{\partial\hat{n}}{\partial t} = \hat{n}\frac{\partial\hat{G}}{\partial t}$

$$\frac{\partial\hat{G}}{\partial t} + \frac{1}{\hat{n}}i\mathbf{k}\cdot\left(\hat{\mathbf{J}}_T - \hat{G}\left\langle\hat{\mathbf{J}}_T\right\rangle_{\theta,r}\right) + \frac{1}{\hat{n}}\nabla_r\cdot\hat{\mathbf{J}}_T + \frac{1}{\hat{n}}\frac{\partial}{\partial\theta}\hat{J}_\theta = 0 \tag{17a}$$

$$\begin{aligned}\frac{1}{\hat{n}}i\mathbf{k}\cdot\left(\hat{\mathbf{J}}_T - \hat{G}\left\langle\hat{\mathbf{J}}_T\right\rangle_{\theta,r}\right) = i\mathbf{k}\cdot(&\\ &U_0\mathbf{u}\hat{G} - \hat{G}U_0\left\langle\mathbf{u}\hat{G}\right\rangle_{\theta,r}\\ &- D_T\left[(i\mathbf{k}+\nabla_r)\hat{G} + \hat{G}\nabla_r\left[\frac{V}{k_{\mathrm{B}}T}\right]\right] + \hat{G}\left[D_T\left(i\mathbf{k}\left\langle\hat{G}\right\rangle_{\theta,r} + \left\langle\nabla_r\hat{G}\right\rangle_{\theta,r} + \left\langle\hat{G}\nabla_r\left[\frac{V}{k_{\mathrm{B}}T}\right]\right\rangle_{\theta,r}\right)\right]\end{aligned} \tag{17b}$$

$$\frac{1}{\hat{n}}(\nabla_r\cdot\hat{\mathbf{J}}_T + \frac{\partial}{\partial\theta}\cdot\hat{J}_\theta) = \nabla_r\cdot\left[U_0\mathbf{u}\hat{G} - D_T\left((i\mathbf{k}+\nabla_r)\hat{G} + \hat{G}\nabla_r\left[\frac{V}{k_{\mathrm{B}}T}\right]\right)\right] + \frac{\partial}{\partial\theta}\left[-D_\theta\left(\frac{\partial}{\partial\theta}\hat{G} + \hat{G}\frac{\partial}{\partial\theta}\left[\frac{V}{k_{\mathrm{B}}T}\right]\right)\right] \tag{17c}$$

$\hat{n}$ only depends on time and wavenumber, so it can be brought into the derivatives and integrals.

After taking advantage of the fact that $\hat{P}/\hat{n} = \hat{G}$, we expand $\hat{G}$ in low wave numbers, and then we group terms in Eq. 17 based on $\mathbf{k}$ order.

$$\hat{G}(\mathbf{k},\mathbf{r},\theta,t) = g(\mathbf{r},\theta,t) + i\mathbf{k}\cdot\mathbf{d}(\mathbf{r},\theta,t) + \mathscr{O}(\mathbf{kk}) \tag{18}$$

The $\mathscr{O}(1)$ term, or the $\mathbf{k}$-independent field g represents the local probability density in a periodic array with identical conditions.

$$\frac{\partial g}{\partial t} + \nabla_r\cdot\mathbf{j}_T^{(0)} + \frac{\partial}{\partial\theta}j_\theta^{(0)} = 0 \tag{19a}$$

$$\mathbf{j}_T^{(0)} = U_0\mathbf{u}g - D_T\left(\nabla_r g + g\nabla_r\left[\frac{V}{k_{\mathrm{B}}T}\right]\right) \tag{19b}$$

$$j_\theta^{(0)} = -D_\theta\left(\frac{\partial}{\partial\theta}g + g\frac{\partial}{\partial\theta}\left[\frac{V}{k_{\mathrm{B}}T}\right]\right) \tag{19c}$$

The $\mathscr{O}(\mathbf{k})$ field $\mathbf{d}$ is the dispersion field. It represents the first correction due to dispersion from to a mild concentration gradient.

$$\frac{\partial \mathbf{d}}{\partial t}+\nabla_r\cdot\mathbf{j}_T^{(1)}+\frac{\partial}{\partial\theta}\mathbf{j}_\theta^{(1)}+U_0\mathbf{u}g-gU_0\left\langle\mathbf{u}g\right\rangle_{\theta,r}-D_T\left[\nabla_r g+g\nabla_r\left[\frac{V}{k_\mathrm{B}T}\right]\right]+gD_T\left[\left\langle\nabla_r g\right\rangle_{\theta,r}+\left\langle g\nabla_r\left[\frac{V}{k_\mathrm{B}T}\right]\right\rangle_{\theta,r}\right]=0 \tag{20a}$$

$$\mathbf{j}_T^{(1)}=U_0\mathbf{u}\mathbf{d}-D_T\left(g\mathbf{I}+\nabla_r\mathbf{d}+\mathbf{d}\nabla_r\left[\frac{V}{k_\mathrm{B}T}\right]\right) \tag{20b}$$

$$\mathbf{j}_\theta^{(1)}=-D_\theta\left(\frac{\partial}{\partial\theta}\mathbf{d}+\mathbf{d}\frac{\partial}{\partial\theta}\left[\frac{V}{k_\mathrm{B}T}\right]\right) \tag{20c}$$

These equations are solved under periodic boundary conditions subject to $\langle g\rangle_{\theta,r}=1$ and $\langle\mathbf{d}\rangle_{\theta,r}=\mathbf{0}$.

Finally, we can relate averages of the local density and fluctuation to transport quantities via the macroscopic density equation:

$$\frac{\partial\hat{n}(\mathbf{k},t)}{\partial t}+i\mathbf{k}\cdot\left\langle\hat{\mathbf{J}}_T\right\rangle_{\theta,r}=0 \tag{21a}$$

$$\left\langle\hat{\mathbf{J}}_T\right\rangle_{\theta,r}=\hat{n}\left[\mathbf{U_E}-i\mathbf{k}\cdot\mathbf{D_E}\right]=\left[U_0\left\langle\mathbf{u}\hat{P}\right\rangle_{\theta,r}-D_T\left(i\mathbf{k}\left\langle\hat{P}\right\rangle_{\theta,r}+\left\langle\nabla_r\hat{P}\right\rangle_{\theta,r}+\left\langle\hat{P}\nabla_r\left[\frac{V}{k_\mathrm{B}T}\right]\right\rangle_{\theta,r}\right)\right] \tag{21b}$$

Replace $\hat{P}=\hat{n}(g+i\mathbf{k}\cdot\mathbf{d}+\ldots)$

$$\left\langle\hat{\mathbf{J}}_T\right\rangle_{\theta,r}=\left[U_0\left\langle\mathbf{u}\hat{n}(g+i\mathbf{k}\cdot\mathbf{d}\right\rangle_{\theta,r}-D_T\left(i\mathbf{k}\left\langle\hat{n}(g+i\mathbf{k}\cdot\mathbf{d})\right\rangle_{\theta,r}+\left\langle\nabla_r\hat{n}(g+i\mathbf{k}\cdot\mathbf{d})\right\rangle_{\theta,r}+\left\langle\hat{n}(g+i\mathbf{k}\cdot\mathbf{d})\nabla_r\left[\frac{V}{k_\mathrm{B}T}\right]\right\rangle_{\theta,r}\right)\right] \tag{22}$$

Factor out $\hat{n}$ and remove the higher order $\mathscr{O}(\mathbf{kk})$ term

$$\hat{n}\left[\mathbf{U_E}-i\mathbf{k}\cdot\mathbf{D_E}\right]=\hat{n}\left[U_0\left\langle\mathbf{u}(g+i\mathbf{k}\cdot\mathbf{d})\right\rangle_{\theta,r}-D_T\left(i\mathbf{k}\left\langle g\right\rangle_{\theta,r}+\left\langle\nabla_r(g+i\mathbf{k}\cdot\mathbf{d})\right\rangle_{\theta,r}+\left\langle(g+i\mathbf{k}\cdot\mathbf{d})\nabla_r\left[\frac{V}{k_\mathrm{B}T}\right]\right\rangle_{\theta,r}\right)\right] \tag{23}$$

Finally, grouping like terms

$$\mathbf{U_E}=\left[U_0\left\langle\mathbf{u}g\right\rangle_{\theta,r}-D_T\left(\left\langle\nabla_r g\right\rangle_{\theta,r}+\left\langle g\nabla_r\left[\frac{V}{k_\mathrm{B}T}\right]\right\rangle_{\theta,r}\right)\right] \tag{24}$$

$$\mathbf{D_E}=D_T\mathbf{I}-\left[U_0\left\langle\mathbf{u}\mathbf{d}\right\rangle_{\theta,r}-D_T\left(\left\langle\nabla_r\mathbf{d}\right\rangle_{\theta,r}+\left\langle\mathbf{d}\nabla_r\left[\frac{V}{k_\mathrm{B}T}\right]\right\rangle_{\theta,r}\right)\right] \tag{25}$$